Robust Optimization Sub-problems and Multicriteria Optimization

Luke E. K. Achenie
(and G. M. Ostrovsky)

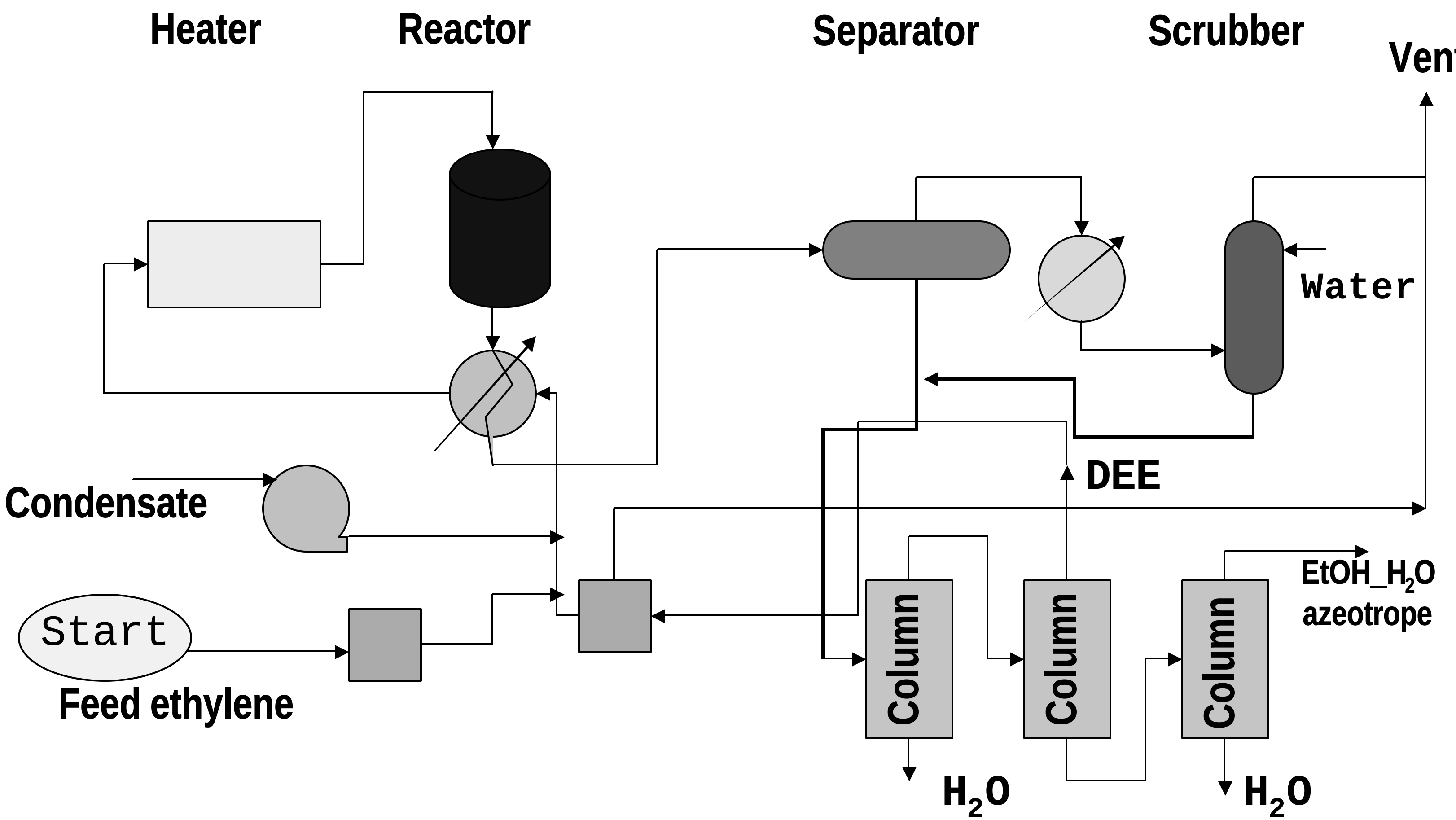
Dept. of Chemical Engineering
University of Connecticut
Storrs, CT

Outline

- Motivational Example - Chemical Process
- Flexibility Concepts
- Feasibility Function Evaluation Methods
- Multicriteria Optimization Under Uncertainty
- Case Studies
- Summary

Example 1: “Large Scale” Chemical Process Flowsheet

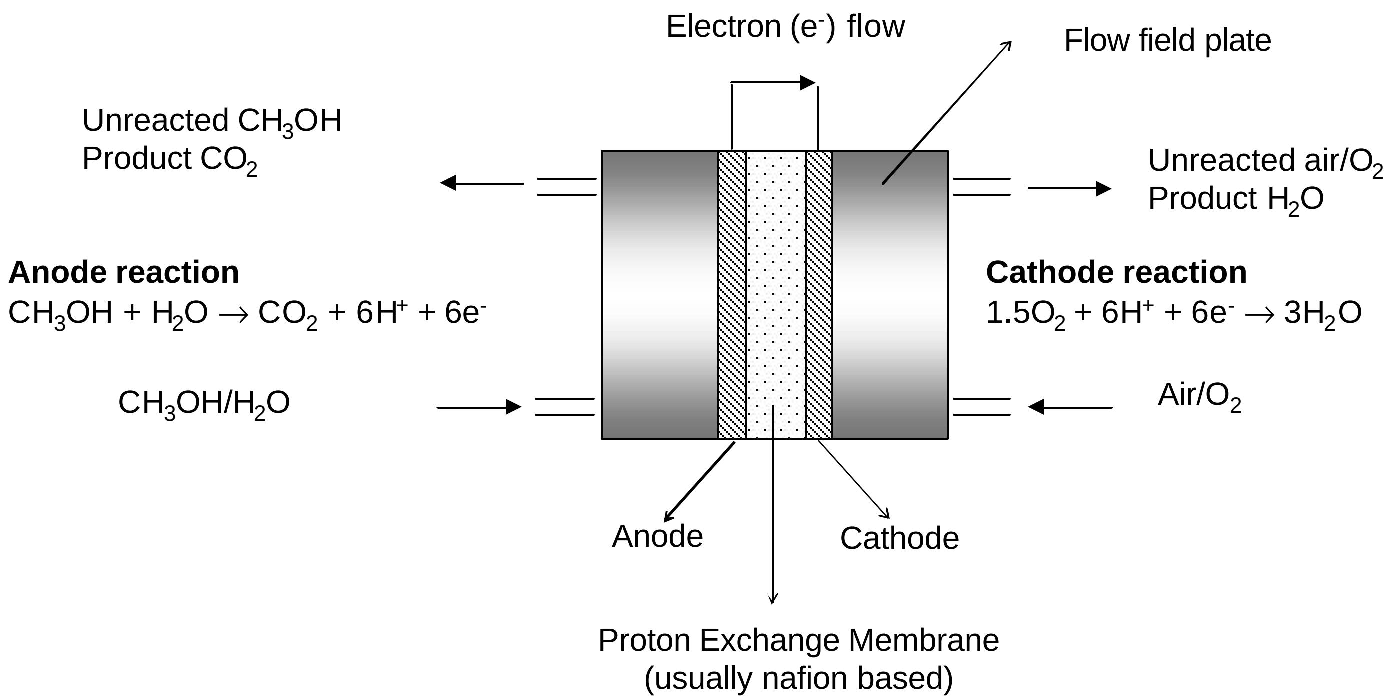
Reaction section



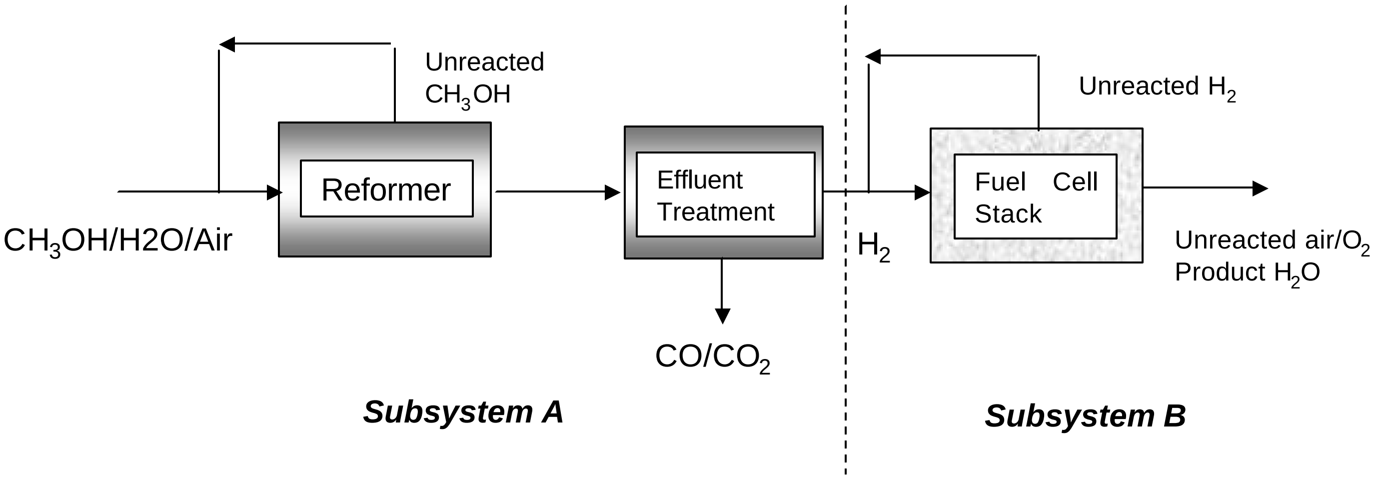
Ethanol Synthesis

Example 2: “Medium Scale” Electrochemical Process

PEM Fuel Cell with Direct Methanol feed

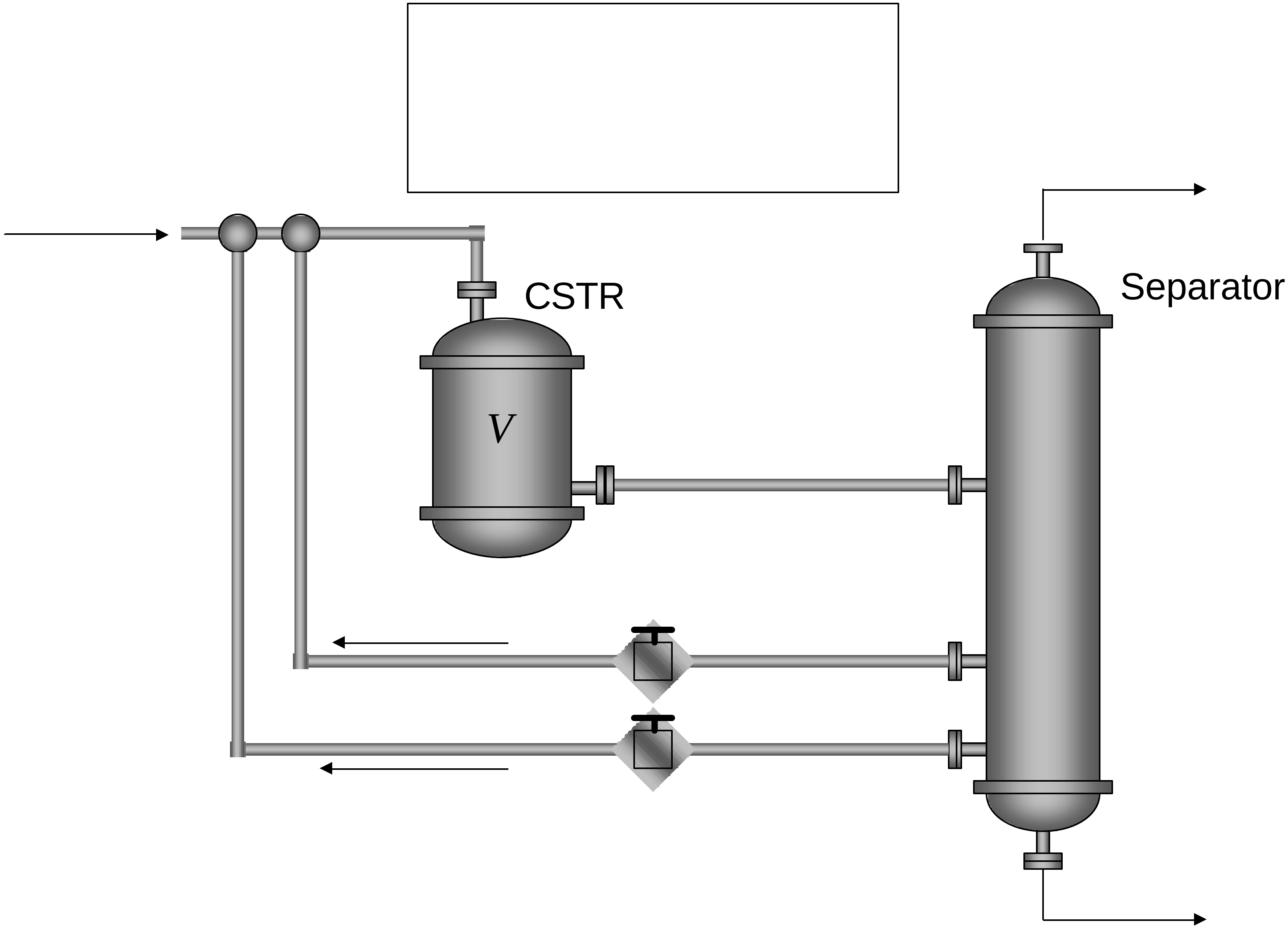


PEM with H_2 feed



Reformer/Fuel Cell System

Example 3: “Small Scale” Chemical Process



Standard Formulation of Optimization Problem

Process
Variables

Uncertain
Parameters

Process Constraints –
material and energy

Process Constraints -
specifications

Re-Formulation of Optimization Problem

Design Variables

Control Variables

State Variables

Sources of Parameteric Uncertainty

- Internal Process Parameters:
  - transfer coefficients, reaction rate constants, activity of catalyst, physical properties, etc.

- External Process Parameters:
  - flow rates, temperature, pressure, environmental specs, cost data, etc.
  - Lag time associated with controller disturbance rejection and set point tracking
  - Geometric uncertainty (e.g. equipment size)

Conditions for Feasible Operation of a Chemical Process (Grossmann et. al.) – see review paper by Sahinidis

$c_1(d)$ is non-differentiable & multi-extremal

$c_1(d)$ £ 0 CP for fixed design d is flexible

$c_1(d) > 0$ CP for fixed design d is not flexible

Two Issues for Feasibility Function

- Problem 1: Is an existing chemical process feasible for fixed design *d* ? Calculate $sign(\chi_1(d)) = \pm$ ➔ *computationally reasonable.*

- Problem 2: What is the value of the feasibility function for a fixed design *d* ? ➔ *computationally intensive*

BB_Active

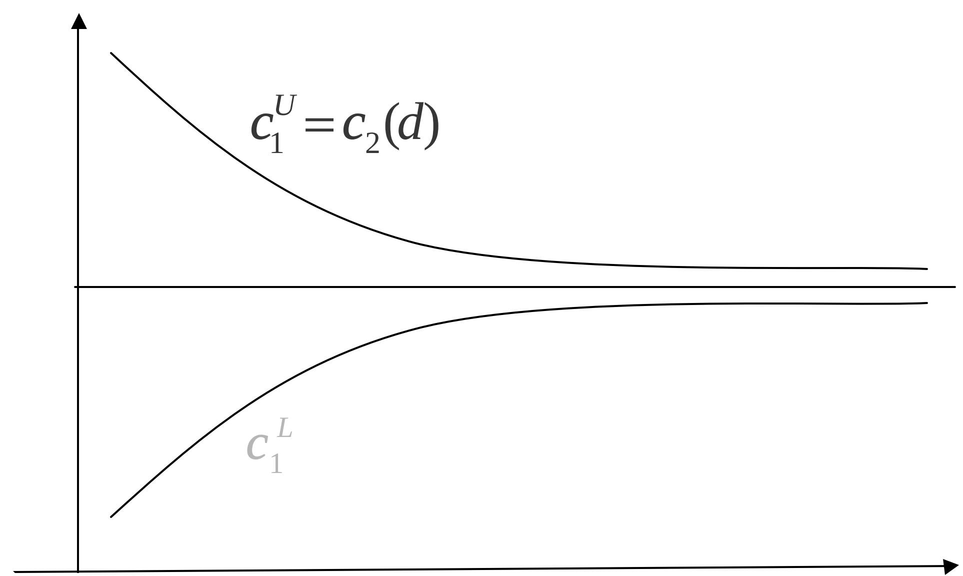
$$c_2(d) = \min_{z} \max_{q \in T} \max_{j} g_j(d, z, q)$$

$$= \min_{z} \max_{j} \max_{q \in T} g_j(d, z, q)$$

$c_2(d)$

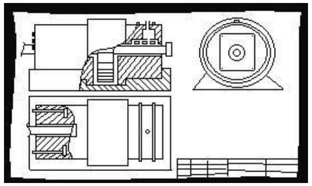
Computationally tractable

Difficult to Evaluate



Typical – Two Stages in the Life of a Chemical Process

Design stage



Operation stage

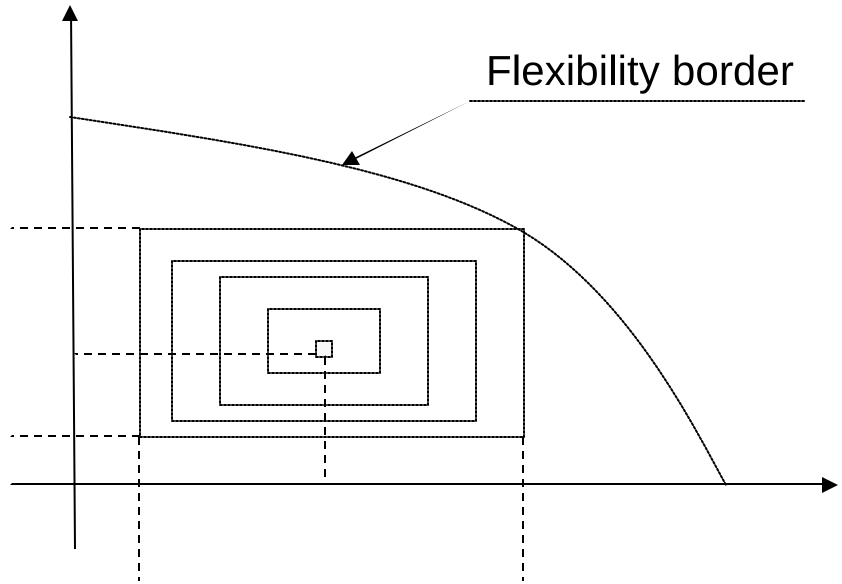
-Design specifications are related to
  - process economics
  - safety
  - environmental

- Control variables can change during both stages

  They can be tuned for satisfaction of the design specifications at each time instant of the operation stage

- Design variables can change only during the ***design*** stage

Main Sub Problems in Flexibility Analysis (I & II)



- determines size of the uncertainty region *T*

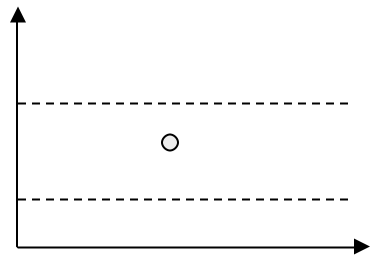
Main Sub Problems in Flexibility Analysis (III)

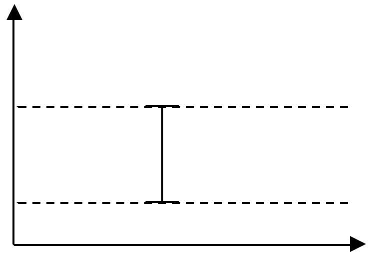
Stochastic programming problem with recourse

Discrete variant through Gaussian quadrature

Uncertainty Types Based on Accuracy

At each time instant during the operation stage, there is at least one uncertain parameter whose accuracy cannot be improved sufficiently using the available process information





<u>Need new formulations for</u>

- Feasibility Test

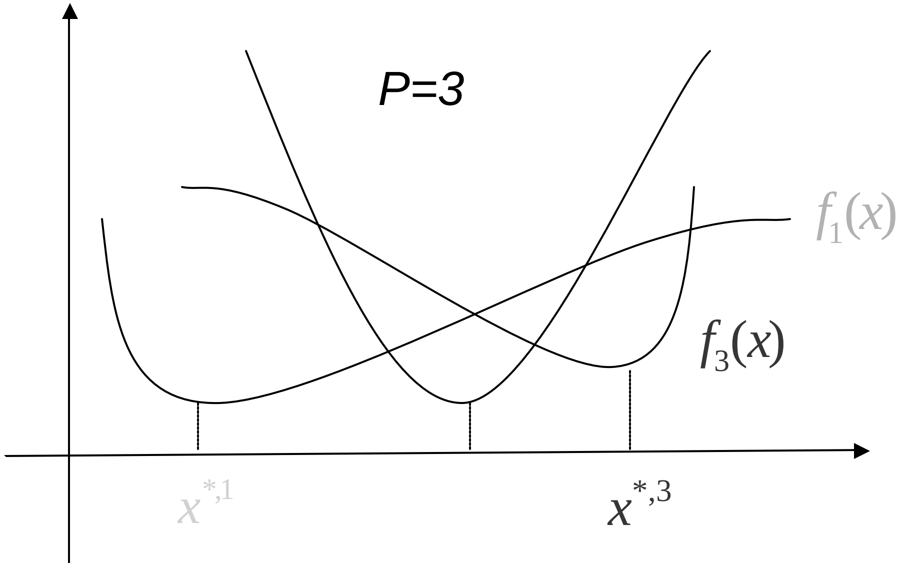
-Two stage optimization problem

- Heat Exchanger Network
- Reactor System

Multicriteria Optimization Under Uncertainty

Multi Criteria Optimization (MCO) – *No Uncertainty*

Solving for each criterion separately



Global minimizers

Which minimizer do we implement? MCO is not well defined as stated!!!

Concepts

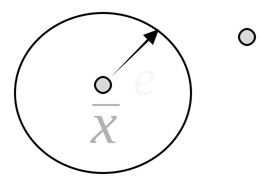
Main concept in MCO

→ Pareto Set (non – inferior set of points)

s.t.

Any point $\bar{x}$

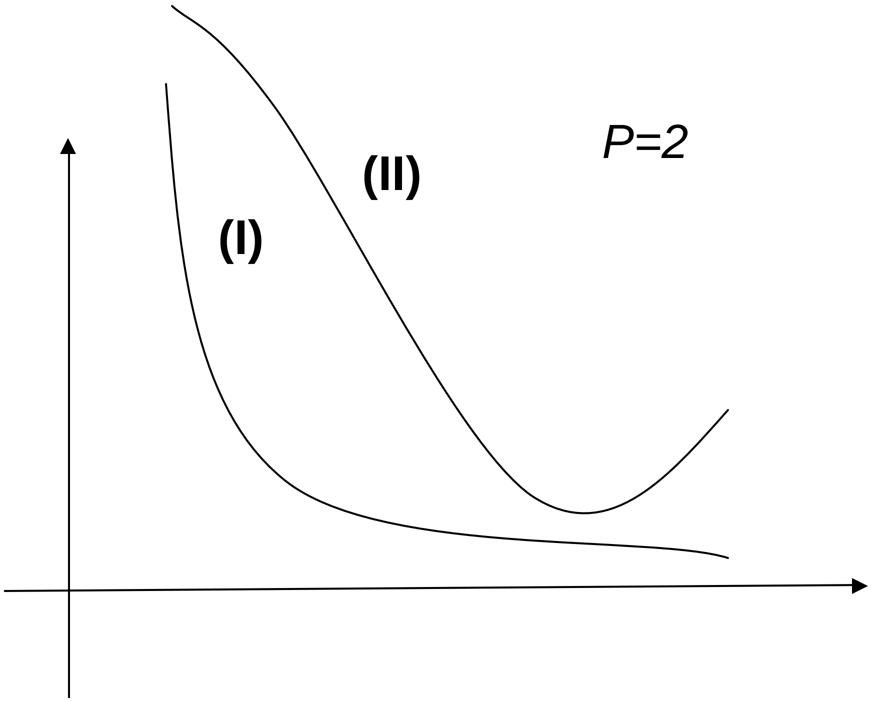
belongs to Pareto Set (PS) if



We cannot find point in which there is at least a j such that

Cannot improve without making another worse

Pareto Set



(I) Pareto Set (II) Not a Pareto Set

Selected Solution Strategies

- Minimization of Average Criterion
- Worst Case Strategy
- Method of Consecutive Conciliations

Multi Criteria Optimization *Under Uncertainty*

How will Pareto Set behave?

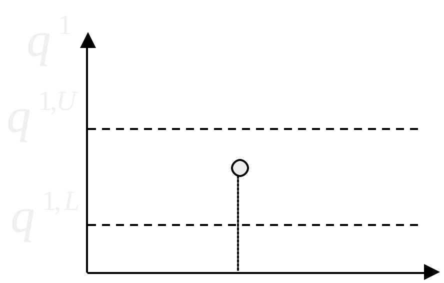
- Case I - One Stage Optimization Problem (OSOP)

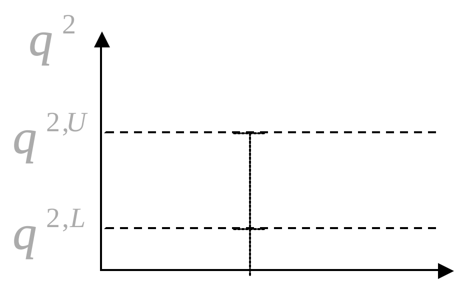
Design and control variables [*d*, *z*] are treated the same

- Case II - Two Stage Optimization Problem (TSOP)

Exploit ability to tune Control variables *z* during operation stage

Two types of uncertain parameters q^1 and q^2





One - Stage MCO problem -- *control variables z cannot be tuned*

Multidimensional
Integrals in θ

Computationally intensive

Scenario 1:

$z^{i*}(d,q)$ = solution of sub-problem for each i

Each has its own $z^{i*}(d,q)$

All $z^{i*}(d,q)$ cannot be realized simultaneously

Cannot implement results

Scenario 2:

Convolution of p criteria for fixed q,

For some set of parameters α construct Pareto Set in the space of design variables d

- Minimization of Average Criteria Example
- Worst Weighted Criterion Example

Case Studies – MCO Under Uncertainty

- ***Direct Methanol Fuel Cell***
- ***Three-Stage Flowsheet***

Optimization Under Uncertainty – Current Large Scale Modeling Efforts (with Biegler)

- ***<u>Direct Methanol Fuel Cell</u>***
- ***<u>Optical Fiber Drawing Process</u>***

Summary

- Feasibility Function Evaluation Methods
- Multicriteria Optimization Under Uncertainty
- Case Studies
- Analysis achievable for small scale plants
- Developing realistic probability functions distribution is necessary but not much effort in this area